

## Sichel model, R code

Bayesian Estimation of Earth's Undiscovered Mineralogical Diversity using Noninformative Priors

Journal of Mathematical Geosciences

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### Estimate the population size  $S$  and the nuisance parameters
### using the Metropolis algorithm for the Sichel distribution

set.seed(99)

library(rstan) #monitoring convergence
library(gsl)   #gsl wrapper for special functions

z=read.delim("TotMinFeb2014.txt")
#Preparing data
attach(z)
count=sort(count,decreasing = TRUE)
N=sum(count)      #Sample size
w=length(count)   #number of distinct minerals
l=unique(count)   #localities
j=rev(l)          #localities ordered
locations=length(l)
nj=numeric(locations) #number of minerals with j localities
for (i in 1:locations){
  nj[i]=length(count[count==j[i]])
}

pen = 1.0e20

# adjusting parameters, smaller values give larger acceptance rate
# stdev for Metropolis algorithm for  $S$ 
st.S = 50

# stdev for Metropolis algorithm for  $a$ 
st.a = 0.01

# stdev for Metropolis algorithm for  $b$ 
st.b = 0.1

# stdev for Metropolis algorithm for  $\gamma$ 
st.gamma = 0.01
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#to monitor acceptance rate
ac=0

#Negative loglikelihood function
negLogLikelihood = function(a, b, gamma, S) {
  if(a <= 0.0 | b <= 0.0){
    return(pen)
  }

  LogFacN=numeric(locations)
  for(i in 1: locations){
    if(j[i]<50) {
      LogFacN[i] = log(fact(j[i]))
    } else {
      LogFacN[i] = lngamma(j[i]+1)
    }
  }
  omega = sqrt(b*b + a*a) - b
  B1=bessel_lnknu(abs(gamma+j), a)
  B2=bessel_lnknu(abs(gamma), omega)
  temp1=j*log((omega*b)/a)
  temp2=gamma*log(omega/a)
  logj=B1-B2+temp1+temp2-LogFacN
  LogP = sum(nj*logj)
  LogPP = LogP - sum(lnfact(nj))
  Log0=bessel_lnknu(abs(gamma),a)-B2+temp2
  Log1 = (S - w)*Log0
  Log2 = - lnfact(S - w)
  Log3 = lnfact(S)
  LogL = LogPP + Log1 + Log2 + Log3
  return(-LogL)
}

#Metropolis algorithm
#Proposal distribution
metropolis=function(a,b,gamma,S,st.a, st.b, st.gamma, st.S){
  a_star=abs(rnorm(1,a,st.a))
  b_star=abs(rnorm(1,b,st.b))
  gamma_star=rnorm(1,gamma,st.gamma)
  repeat{
    S_star=floor(abs(rnorm(1,S,st.S)))
    if(S_star>w-1)
      break
  }
  logr=negLogLikelihood(a,b,gamma,S)-negLogLikelihood(a_star,b_star,gamma_star,S_star)
}

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r=exp(logr)
# accept or reject proposed value
if (runif(1)<min(r,1)){a=a_star; b=b_star; gamma=gamma_star; S=S_star; ac=ac+1}
else{
  a=a; b=b; gamma=gamma; S=S; ac=ac
}
return(c(a=a, b=b, gamma=gamma, S=S, ac=ac))
}

#Number of chains
chains = 3
#Number of iterations
iter = 1000000

simulations = array(NA, c(iter, chains, 4))
dimnames(simulations) = list(NULL, NULL, c("a","b","gamma", "S"))
for (kk in 1:chains){
  # starting values
  a=0.08+(kk-1)*2*st.a
  b=0.8+(kk-1)*2*st.b
  gamma=-0.52+(kk-1)*2*st.gamma
  S=6118+(kk-1)*2*st.S
  for (t in 1:iter){
    temp = unlist(metropolis(a,b,gamma,S,st.a, st.b, st.gamma, st.S))
    a = as.numeric(temp[1])
    b = as.numeric(temp[2])
    gamma = as.numeric(temp[3])
    S = as.numeric(temp[4])
    ac = as.numeric(temp[5])
    simulations[t,kk,] <- c(a,b,gamma,S)
  }
}
monitor(simulations,digit=4)

```